

5-Methyl-1-phenylpyrazole-4-carboxylic acid

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|-----------------------------|--|
| Inchi: | InChI=1S/C11H10N2O2/c1-8-10(11(14)15)7-12-13(8)9-5-3-2-4-6-9/h2-7H,1H3,(H,14,15) |
| InchiKey: | USSMIQWDLWJQDQ-UHFFFAOYSA-N |
| Formula: | C11H10N2O2 |
| SMILES: | Cc1c(C(=O)O)cnn1-c1ccccc1 |
| Mol. weight [g/mol]: | 202.21 |
| CAS: | 91138-00-0 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.43 | | Crippen Method |
| logp | 1.879 | | Crippen Method |
| mcvol | 150.030 | ml/mol | McGowan Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C91138000&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

| | |
|-----------------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |

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